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Supporting Information to Theoretical screening of Co- and Mo- based binary alloys for interconnect metal

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Table S1. Material properties used and calculated shown in Fig. 3-(a) (*Co* based binary alloys). Values omitted has more than 40 atoms per unit cell, which were screened out by process shown in Fig. 1

Material ID (material project)	Formula	Crystal System	Space Group	Atoms / Cell	Total Magnetization	Spin Polarized	Cohesive Energy	FoM
mp-493	Co2B	Tetragonal	I4/mcm	6	4.03	O	5.82214955	7.438072
mp-20857	CoB	Orthorhombic	Pnma	8	0.00	X	6.188115263	118.974300
mp-20373	Co3B	Orthorhombic	Pnma	16	14.26	O	5.656889941	12.412704
mp-639154	Co23B6	Cubic	Fm3¯m	29	35.16	O	5.567709214	13.750494
mp-1194572	Co5B16	Orthorhombic	Pmma	42	0.03	X	6.27494412	*
mp-22488	Co2C	Orthorhombic	Pnnm	6	0.00	X	5.987984768	9.659556
mp-20925	Co3C	Orthorhombic	Pnma	16	12.33	O	5.732168475	11.666706
mp-1272749	CoO2	Trigonal	R-3m	6	2.00	O	5.070962102	25.82042
mp-796278	CoO2	Orthorhombic	Cmce	6	2.00	O	4.91327664	15.467964
mp-32686	CoO2	Trigonal	P-3m1	6	0.00	X	5.069236228	10.26817
mp-19079	CoO	Cubic	Fm-3m	4	6.00	O	5.535362893	9.72871
mp-18748	Co3O4	Cubic	Fd-3m	14	6.00	O	5.453744253	9.72871
mp-550206	CoO2	Trigonal	R-3m	3	1.00	O	11.81295099	16.162792
mp-1062643	CoO2	Orthorhombic	Fmm2	3	2.66	O	4.556901533	13.154472
mp-556750	CoO2	Monoclinic	C2/m	3	1.00	O	4.91454225	42.58972
mp-1062939	CoO2	Trigonal	R-3m	12	4.00	O	5.06910442	19.477516
mp-823	TiCo	Cubic	Pm3¯m	2	0.87	O	5.827290455	5.056102
mp-608	TiCo3	Cubic	Pm3¯m	4	2.77	O	5.555724798	6.053628
mp-30566	Ti2Co	Cubic	Fd3¯m	6	2.40	O	5.075543827	9.139148
mp-695	TiCo2	Cubic	Fd3¯m	6	4.06	O	5.640645908	7.049142
mp-1191331	Ti2Co	Cubic	Fd3¯m	24	0.00	X	5.800173198	17.326530
mp-1191422	TiCo2	Hexagonal	$P6_3/mmc$	24	15.97	O	5.64306793	14.474858
mp-1585	V3Co	Cubic	Pm3¯n	8	0.00	X	5.551537319	12.676610
mp-542614	VCo3	Hexagonal	$P6_3/mmc$	24	0.02	O	5.39843984	12.152410
mp-2283	ZrCo	Cubic	Pm3¯m	2	1.00	O	6.124773575	6.14922
mp-628	Zr2Co	Tetragonal	I4/mcm	6	0.00	X	6.31432221	11.215560
mp-929	ZrCo2	Cubic	Fd3¯m	6	4.03	O	5.920542678	8.362518
mp-1079065	Zr3Co	Hexagonal	$P6_3/mcm$	8	0.02	O	6.048112834	14.563028
mp-30619	Zr3Co	Orthorhombic	Cmcm	8	0.00	X	6.379708908	13.383880
mp-1191437	Zr2Co	Cubic	Fd3¯m	24	0.00	X	6.255199776	24.630140
mp-30569	Zr6Co23	Cubic	Fm3¯m	29	32.59	O	5.664036032	24.391320
mp-670	NbCo2	Cubic	Fd3¯m	6	6.63	O	5.90796653	7.507712
mp-1101983	NbCo2	Hexagonal	$P6_3/mmc$	12	1.95	O	5.906675183	10.81935
mp-7250	Nb6Co7	Trigonal	R3¯m	13	1.12	O	6.158897049	16.835792
mp-1104334	Nb7Co6	Trigonal	R3¯m	13	0.00	X	6.307122538	12.832480
mp-1191009	NbCo2	Hexagonal	$P6_3/mcm$	24	29.56	O	5.911847308	11.566010
mp-570557	NbCo3	Hexagonal	$P6_3mc$	24	11.59	O	5.706320553	15.107302
mp-1139	Co3Mo	Hexagonal	$P6_3/mmc$	8	3.95	O	5.484417184	15.114846
mp-567747	Co7Mo6	Trigonal	R3¯m	13	1.34	O	5.686891813	12.953006
mp-2027	HfCo	Cubic	Pm3¯m	2	0.96	X	6.364851	8.350000
mp-1064981	HfCo	Orthorhombic	Cmcm	4	0.61	X	6.367473	9.270024
mp-2337	HfCo2	Cubic	Fd3¯m	6	4.06	O	6.067184	8.016294
mp-1205422	Hf2Co7	monoclinic	C12/m1	18	15.46	O	5.774103	12.908588
mp-1190841	Hf2Co	Cubic	Fd3¯m	24	0.00	X	6.5267	27.451920
mp-1192795	Hf6Co23	Cubic	Fd3¯m	29	32.62	O	5.742836	25.599280
mp-11358	TaCo3	Cubic	Pm3¯m	4	1.88	O	6.215700838	9.831698
mp-574	Ta2Co	Tetragonal	I4/mcm	6	0.00	X	7.591514793	12.494540
mp-1799	TaCo2	Cubic	Fd3¯m	6	2.19	O	6.468913833	7.01185
mp-1102370	Ta2Co	Hexagonal	$P6_3/mcm$	12	0.00	O	7.122409092	15.620246
mp-570430	TaCo2	Hexagonal	$P6_3/mcm$	12	12.61	O	6.464924354	10.65236
mp-7851	TaCo3	Trigonal	R3¯m	12	0.02	O	6.217847381	11.016988
mp-1104548	Ta7Co6	Trigonal	R3¯m	13	0.00	X	7.174329632	11.725780
mp-570463	TaCo2	Hexagonal	$P6_3/mmc$	24	0.07	O	6.471131494	13.356362
mp-2157	Co3W	Hexagonal	$P6_3/mmc$	8	3.55	O	6.0305707	14.305044
mp-1105377	Co7W6	Trigonal	R3¯m	13	13.01	O	4.401956737	13.647884
mp-949	CoPt	Tetragonal	P4/mmm	4	4.82	O	2.096208988	6.289098
mp-922	CoPt3	Cubic	Pm-3m	4	2.85	O	5.495491588	5.197274

Table S2. Same as Table S1 but for *Mo* based binary alloys.

Material ID (material_project)	Formula	Crystal System	Space Group	Atoms / Cell	Total Magnetization	Spin Polarized	Cohesive Energy	FoM
mp-11271	BeMo3	Cubic	Pm-3n	8	0.01	X	5.611166128	13.103900
mp-1677	Be2Mo	Hexagonal	P6_3/mmc	12	0.00	X	4.882151769	14.867340
mp-1475	Be12Mo	Tetragonal	I4/mmm	13	0.00	X	4.043525872	21.116670
mp-30440	Be22Mo	Cubic	Fd-3m	46	0.00	X	3.883657726	*
mp-2501	BMo2	Tetragonal	I4/mcm	6	0.00	X	6.615547053	7.795812
mp-7229	B5Mo2	Trigonal	R-3m	7	0.02	X	6.297480357	6.695003
mp-960	B2Mo	Hexagonal	P6/mmm	3	0.00	X	6.630541043	5.166381
mp-999198	BMo	Orthorhombic	Cmcm	4	0.00	X	6.819283928	7.100315
mp-1079053	B2Mo3	Tetragonal	P4/mbm	10	0.00	X	6.680537762	8.931955
mp-2331	B2Mo	Trigonal	R-3m	6	0.00	X	6.786645975	8.550220
mp-1890	BMo	Tetragonal	I4_1/amd	8	0.00	X	6.82922139	10.094240
mp-1106346	B4Mo	Hexagonal	P6_3/mmc	20	0.02	X	6.104011342	9.513375
mp-567925	MoC	Hexagonal	P6_3/mmc	8	0.00	X	6.975651073	7.638355
mp-2305	MoC	Hexagonal	P-6m2	2	0.00	X	7.188843365	16.34503
mp-15798	MoC	Hexagonal	P6_3/mmc	12	0.00	X	6.935326344	11.58021
mp-1552	Mo2C	Orthorhombic	Pbcn	12	0.00	X	6.930890817	10.55322
mp-2746	MoC	Cubic	Fm-3m	2	0.00	X	6.891940615	4.962308
mp-27953	Mo2N	Tetragonal	I4_1/amd	6	0.00	X	6.264377955	7.704012
mp-2811	MoN	Hexagonal	P6_3mc	16	0.00	X	6.281076626	13.861980
mp-1065394	MoN	Hexagonal	P6_3/mmc	4	0.00	X	6.26723319	5.611238
mp-2355	MoN	Hexagonal	P6/mmm	4	0.00	X	4.420232623	7.772613
mp-1078389	MoN	Hexagonal	P6_3/mmc	8	0.00	X	6.270743293	7.653668
mp-1064706	MoN	Orthorhombic	Imma	4	0.00	X	5.522661465	20.352220
mp-1180348	Mo3O10	Hexagonal	P6_3/m	26	0.39	O	5.69141449	50.9618
mp-540786	Mo4O11	Orthorhombic	Pnma	60	7.97	*	6.108272729	*
mp-1180281	Mo3O10	Orthorhombic	Aea2	26	4.00	O	5.657635432	*
mp-510536	MoO2	Tetragonal	P4_2/mnm	12	8.00	O	1.911253491	*
mp-559140	MoO2	Monoclinic	P2_1/c	12	0.00	X	6.184943998	29.811890
mp-285	Mo17O47	Orthorhombic	Pba2	128	16.18	*	6.103563334	*
mp-542610	Mo4O11	Orthorhombic	Pna2_1	60	8.00	*	6.100626285	*
mp-28777	Mo9O25	Monoclinic	P2/c	68	8.00	*	6.099777846	*
mp-30544	Mo5O14	Monoclinic	P2_1/c	76	8.00	*	6.094273635	*
mp-550	Al12Mo	Cubic	Im-3	13	0.00	X	3.857414786	22.90041
mp-568153	Al22Mo5	Orthorhombic	Fdd2	54	0.00	X	4.290925027	*
mp-1198386	Al2Mo3	Monoclinic	P2_1/c	40	0	*	5.092649731	*
mp-30180	Al4Mo	Monoclinic	Cm	15	0.01	X	4.323638093	36.386890
mp-259	AlMo3	Cubic	Pm-3n	8	0.00	X	5.808786616	14.839340
mp-571053	Al5Mo	Trigonal	R-3c	12	0.00	X	4.219873669	21.415300
mp-568607	Al5Mo	Hexagonal	P6_322	12	0.00	X	4.224137604	25.379870
mp-2733	Al8Mo3	Monoclinic	C2/m	11	0.00	X	4.605148065	227.534000
mp-569049	Al5Mo	Trigonal	P321	60	0.02	*	4.222309619	*
mp-2592	Si2Mo	Tetragonal	I4/mmm	3	0.00	X	5.645199247	50.156905
mp-1275	SiMo3	Cubic	Pm-3n	8	0.00	X	6.146577639	9.753206
mp-1332	Si3Mo5	Tetragonal	I4/mcm	16	0.00	X	6.000473887	15.599660
mp-1188373	Si3Mo5	Hexagonal	P6_3/mcm	16	0.03	X	5.905973654	13.535900
mp-1087230	Si2Mo3	Tetragonal	P4/mbm	10	0.00	X	5.825280674	11.003600
mp-10004	Mo3P	Tetragonal	I-42m	16	0.00	X	5.91362705	17.279740
mp-1189099	Mo3P	Tetragonal	I-4	16	0.02	X	5.912708083	*
mp-21833	Mo4P3	Orthorhombic	Pnma	56	0.01	X	5.632871706	*
mp-1237770	Mo12P	Trigonal	R3	26	0.13	O	5.66542936	*
mp-27413	Mo8P5	Monoclinic	Pm	13	0.00	X	5.690775105	18.571680
mp-1887	MoP2	Orthorhombic	Cmc2_1	6	0.00	X	4.946772975	48.220090
mp-219	MoP	Hexagonal	P-6m2	2	0.00	X	5.539897205	10.935020
mp-11508	MoP4	Monoclinic	C2/c	10	0.00	X	4.400315146	120.817100
mp-1194842	Mo12P	Trigonal	R3	26	0.00	X	5.634671078	36.925000
mp-1627	Mo2S3	Monoclinic	P2_1/m	10	0.02	X	5.43056469	21.263950
mp-2164	Mo3S4	Trigonal	R-3	14	0.00	X	5.495439812	112.935700
mp-31257	Mo15S19	Hexagonal	P6_3/m	68	0.00	X	5.493160698	*
mp-558544	MoS2	Trigonal	R-3m	3	0.00	X	5.166714237	24.112770
mp-1104577	Mo3S4	Triclinic	P-1	14	0.01	X	5.449809927	23.429660
mp-1193426	Fe25Mo4	Cubic	I-43m	29	43.38	O	5.125397683	24.520440
mp-569594	Fe7Mo6	Trigonal	R-3m	13	8.00	O	5.600814866	12.106788
mp-1095682	Fe2Mo	Hexagonal	P6_3/mmc	12	5.14	O	5.453373316	12.844470
mp-1139	Co3Mo	Hexagonal	P6_3/mmc	8	3.95	O	5.484417184	15.107302
mp-567747	Co7Mo6	Trigonal	R-3m	13	1.34	O	5.686891813	15.114846
mp-2377	GaMo3	Cubic	Pm-3n	8	0.00	X	5.524561424	13.219270
mp-1203833	Ga31Mo6	Triclinic	P-1	74	0.00	*	3.40957608	*

mp-1203833	Ga31Mo6	Triclinic	P-1	74	0.00	*	3.40957608	*
mp-569901	Ge23Mo13	Tetragonal	P-4n2	144	0.04	*	4.77472349	*
mp-13688	Ge2Mo	Orthorhombic	Pnma	12	0.00	X	4.743658821	7.731149
mp-17094	Ge3Mo5	Tetragonal	I4/mcm	16	0.00	X	5.419990433	16.869620
mp-494	GeMo3	Cubic	Pm-3n	8	0.00	X	5.768351262	9.531251
mp-10201	Ge2Mo	Tetragonal	I4/mmm	3	0.00	X	4.723361223	43.157750
mp-2049	ZrMo2	Cubic	Fd-3m	6	0.00	X	6.469744307	11.450820
mp-30790	ZrMo3	Cubic	Pm-3n	8	0.00	X	6.08095667	10.596680
mp-1193202	Mo2Ru	Tetragonal	P4_2/mnm	30	0.01	X	6.51838373	15.537350
mp-30787	MoRh3	Hexagonal	P6_3/mmc	8	0.00	X	6.30044481	8.769878
mp-12595	MoRh	Orthorhombic	Pmma	4	0.00	X	6.313643472	6.366194
mp-2363	HfMo2	Cubic	Fd-3m	6	0.00	X	6.591060957	11.505120
mp-1191083	HfMo2	Hexagonal	P6_3/mmc	24	0.00	X	6.584204953	14.282500
mp-1103318	MoW11	Orthorhombic	Pmmm	12	0.00	X	6.417984239	6.554230
mp-12662	Re24Mo5	Cubic	I-43m	29	0.00	X	7.498552637	24.089380
mp-801	Mo3Os	Cubic	Pm-3n	8	0.00	X	6.753689792	7.735607
mp-11481	MoIr	Orthorhombic	Pmma	4	0.00	X	7.058414552	6.433847
mp-11482	MoIr3	Hexagonal	P6_3/mmc	8	0.00	X	7.313762063	9.121569
mp-1120	Mo3Ir	Cubic	Pm-3n	8	0.04	X	6.585773151	8.353028
mp-952	MoPt2	Orthorhombic	Immm	3	0.00	X	6.12976876	*
mp-999502	MoPt	Orthorhombic	Pmma	4	0.00	X	6.207854495	8.939959
mp-1232	Mo3Pt	Cubic	Pm-3n	8	0.00	X	6.178667495	9.275386